Amendment to the Specification

Please amend the Abstract as follows:

Abstract

A method for segregating compounds by ionization polarity by: a) selecting a data base of a statistically significant group of compounds and determining the polarization at which each ~~of said~~ compounds ~~is~~ ionized; b) structurally analyzing the individual compounds to determine structural characteristics common to a majority of compounds which ionize at each polarity to determine structural characteristics common structural characteristics, as polarization determinants; c) sequentially arranging the polarization determinants in classification trees according to percentage determination of polarization; d) applying the polarization determinants in classification trees in classifying a new compound for a predicted polarization of positive or negative at which ~~said~~ the compound is ionized; e) segregating compounds classified as ionizing at positive polarity and compounds classified as ionizing at negative polarity; and f) separately analyzing the segregated compounds with the respective predicted polarities with an analysis instrument operable in different modes depending on ionization polarity.

Please amend the specification at page 3, lines 23-37, (paragraph 0025 of the published application), as indicated:

[0025] As shown in Figure 1, starting at the top of the tree, there are 698 starting compounds which were analyzed for polarity during ionization, 74% of which were ionized at a positive polarity. The compounds are separated into two groups 2a and 2b, depending on whether an OH group is present (+) of absent (-). The 210 compounds with an OH group present are less likely to be ionized at positive polarity (38%), while the 488 compounds without an OH group drop down the tree to the left and are much more likely to be ionized at positive polarity (90%). The two groups are then further segregated based on the best discriminating factor for the particular group. The 210 compounds with an OH group present are divided based on whether there are more than two oxygen atoms present. Compounds with more than two oxygen atoms are less likely to be ionized at positive polarity (23%). In contrast, compounds with less than two oxygen atoms present are more likely to be ionized at positive polarity. Every compound in all of the groups ends up in one of the four bottom leaves 3a-d of the tree with the percentages in the respective leaves serving as predictions regarding how likely a compound with the

particular structural set of discriminator structural elements will be ionized at positive polarity.